Abstract

MOLECULAR MODELING FOR METALLOPROTEINS

A method for designing a metal ion for use in a MD simulation can include the steps of building a metal ion molecule having a center atom and a dummy atom, assigning a van der Waals radius to the center atom, and assigning a charge to the dummy atom. A metal ion molecule can have. The center atom covalently linked to one or more dummy atoms resulting in the metal ion molecule having a polyhedron geometry. New force field parameters may be used in methods for designing metal ions for use in MD simulations.